EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	709	514/252.16.ccls.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/23 13:24
L2	2	pyrazolopyrimidinethione	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/23 13:30
L3	1	l1 and l2	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/23 13:25
S1	4	((SHUXIN) near2 (LI)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/23 13:21
S2	9	((JIANPING) near2 (REN)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:20
S3	1	((YANJIN) near2 (ZHAO)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:20
S4	1	((QIUJUN) near2 (LV)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:20
S5	1	((JINHUA) near2 (GUO)).INV.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:43
S6	2	("6200782"|"6350751").PN.	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:44
S7	1407	pyrazolopyrimidine$	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:45
S8	1398	pyrazolopyrimidine	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:44
S9	14	S1 S2 S3 S4 S5 S6	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:44
S10	1	S7 and S9	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:44
S11	0	S8 and S9	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:44
S12	2	pyrazolopyrimidinethione$	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:45

EAST Search History

S13	2	pyrazolopyrimidinethione	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:45
S14	1	S12 and S9	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:45
S15	1	S13 and S9	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/22 11:45
S16	0	"204152709"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/23 10:25
S17	0	"2004152709"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/23 10:25
S18	1	"20040152709"	US-PGPUB; USPAT; USOCR	OR	ON	2007/10/23 10:25

CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:02:47 ON 23 OCT 2007

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:03:14 ON 23 OCT 2007
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STRUCTURE FILE UPDATES: 21 OCT 2007 HIGHEST RN 951124-19-9
DICTIONARY FILE UPDATES: 21 OCT 2007 HIGHEST RN 951124-19-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

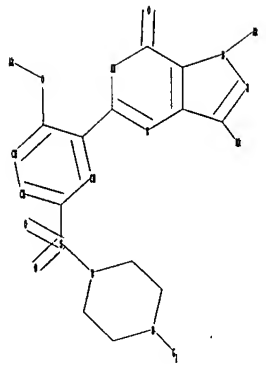
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

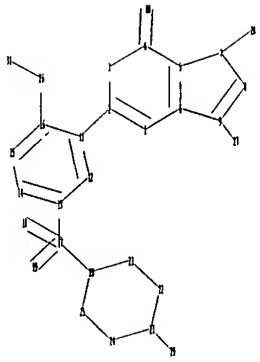
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10583335\10583335b.str



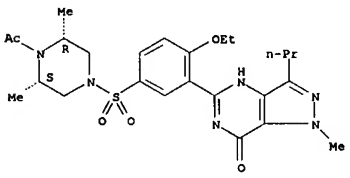


chain nodes :
10 17 18 19 26 27 28 29 31
ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 20 21 22 23 24 25
chain bonds :
2-11 4-10 7-28 9-27 13-17 16-26 17-18 17-19 17-20 23-29 26-31
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-16 12-13 13-14 14-15
15-16 20-21 20-25 21-22 22-23 23-24 24-25
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-10 5-6 5-7 6-9 7-8 7-28 8-9 9-27 13-17 16-26
17-18 17-19 17-20 20-21 20-25 21-22 22-23 23-24 23-29 24-25 26-31
exact bonds :

```
2-11
normalized bonds :
11-12  11-16  12-13  13-14  14-15  15-16


G1:H,Ak,Cb

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:CLASS  18:CLASS  19:CLASS
20:Atom  21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:CLASS  27:CLASS  28:CLASS
29:CLASS  31:CLASS



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 10:03:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       89 TO ITERATE

100.0% PROCESSED       89 ITERATIONS                                 9 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          1214 TO     2346
PROJECTED ANSWERS:                9 TO      360

L2             9 SEA SSS SAM L1

=> d scan
```

L2 9 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Piperazine, 1-acetyl-4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-2,6-dimethyl-, (2R,6S)-rel- (9CI)
MF C25 H34 N6 O5 S

Relative stereochemistry.



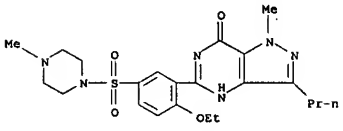
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

```
=> s l1 full
FULL SEARCH INITIATED 10:04:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      1639 TO ITERATE

100.0% PROCESSED      1639 ITERATIONS                                  218 ANSWERS
SEARCH TIME: 00.00.01

L3           218 SEA SSS FUL L1

=> d scan
```

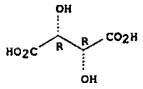
L3 218 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C22 H30 N6 O4 S . 1/2 C4 H6 O6

CM 1



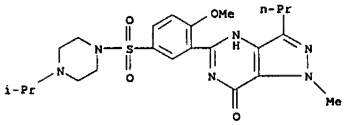
CM 2

Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

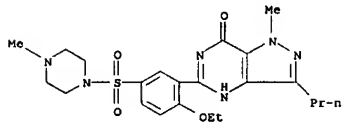
L3 218 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 1,6-dihydro-5-[2-methoxy-5-[[4-(1-methylethyl)-1-piperazinyl]sulfonyl]phenyl]-1-methyl-3-propyl-
MF C23 H32 N6 O4 S



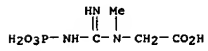
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 218 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Glycine, N-[imino(phosphonoamino)methyl]-N-methyl-, compd. with 5-[2-ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one (1:1)
MF C22 H30 N6 O4 S . C4 H10 N3 O5 P

CM 1



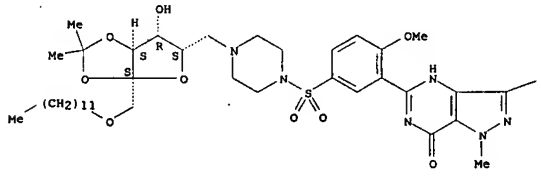
CM 2



L3 218 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN α-L-Sorbofuranose, 6-deoxy-6-[4-[[3-(6,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-methoxyphenyl]sulfonyl]-1-piperazinyl]-1-O-dodecyl-2,3-O-(1-methylethylidene)-, hydrochloride (1:1)
MF C41 H64 N6 O9 S . Cl H

Absolute stereochemistry.

PAGE 1-A



● HCl

PAGE 1-B

Pr-n

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

```
=> file caplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       172.55     172.76

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FILE COVERS 1907 - 23 Oct 2007  VOL 147 ISS 18
FILE LAST UPDATED: 22 Oct 2007  (20071022/ED)

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http://www.cas.org/infopolicy.html

=> s l3
L4         1875 L3

=> s l3 not pd>20031218
           1875 L3
        4864415 PD>20031218
                (PD>20031218)
L5          650 L3 NOT PD>20031218

=> file registry
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         3.42     176.18

FILE 'REGISTRY' ENTERED AT 10:06:07 ON 23 OCT 2007
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STRUCTURE FILE UPDATES:   21 OCT 2007  HIGHEST RN 951124-19-9
DICTIONARY FILE UPDATES:  21 OCT 2007  HIGHEST RN 951124-19-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
```
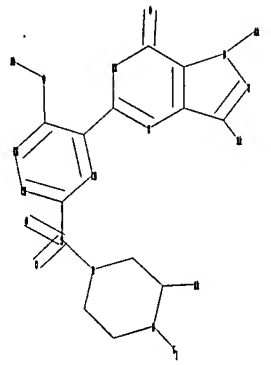
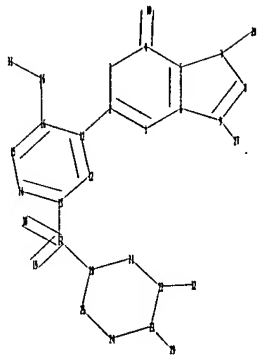

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10 series\10583335\10583335c.str



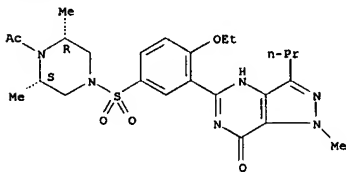


chain nodes :
10 17 18 19 26 27 28 29 31 32
ring nodes :
1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 20 21 22 23 24 25

```
chain bonds :
2-11  4-10  7-28  9-27  13-17  16-26  17-18  17-19  17-20  22-32  23-29  26-31
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9  11-12  11-16  12-13  13-14  14-15
 15-16  20-21  20-25  21-22  22-23  23-24  24-25
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  4-10  5-6  5-7  6-9  7-8  7-28  8-9  9-27  13-17  16-26
17-18  17-19  17-20  20-21  20-25  21-22  22-23  22-32  23-24  23-29  24-25  26-31
exact bonds :
2-11
normalized bonds :
11-12  11-16  12-13  13-14  14-15  15-16


G1:H,Ak,Cb

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:CLASS  18:CLASS  19:CLASS
20:Atom  21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:CLASS  27:CLASS  28:CLASS
29:CLASS  31:CLASS  32:CLASS



L6      STRUCTURE UPLOADED

=> d l6
L6 HAS NO ANSWERS
L6              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l6
SAMPLE SEARCH INITIATED 10:06:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       89 TO ITERATE

100.0% PROCESSED       89 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1214 TO     2346
PROJECTED ANSWERS:               1 TO       80

L7            1 SEA SSS SAM L6

=> d scan
```

L7 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Piperazine, 1-acetyl-4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-2,6-dimethyl-, (2R,6S)-rel- (9CI)
MF C25 H34 N6 O5 S

Relative stereochemistry.



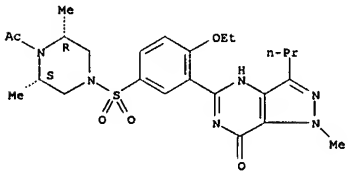
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

```
=> s l6 full
FULL SEARCH INITIATED 10:07:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      1639 TO ITERATE

100.0% PROCESSED     1639 ITERATIONS                                  6 ANSWERS
SEARCH TIME: 00.00.01

L8             6 SEA SSS FUL L6

=> d scan
```

L8 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Piperazine, 1-acetyl-4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-2,6-dimethyl-, (2R,6S)-rel- (9CI)
MF C25 H34 N6 O5 S

Relative stereochemistry.

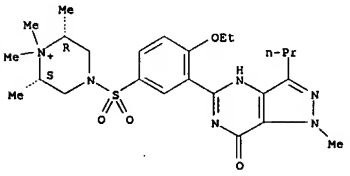


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

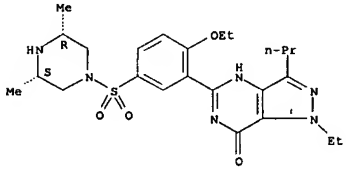
L8 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Piperazinium, 4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1,1,2,6-tetramethyl-, (2R,6S)-rel- (9CI)
MF C25 H37 N6 O4 S

Relative stereochemistry.



L8 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Piperazine, 1-[[4-ethoxy-3-(1-ethyl-4,7-dihydro-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel- (9CI)
MF C24 H34 N6 O4 S

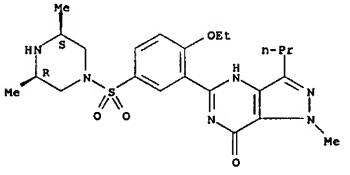
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 6 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
MF C23 H32 N6 O4 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	348.73

FILE 'CAPLUS' ENTERED AT 10:07:26 ON 23 OCT 2007
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FILE COVERS 1907 - 23 Oct 2007 VOL 147 ISS 18
FILE LAST UPDATED: 22 Oct 2007 (20071022/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

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=> s l8
L9 8 L8

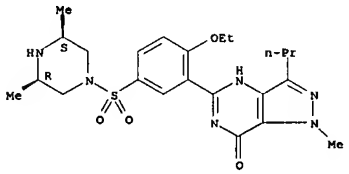
=> d l9 1-8 ibib abs hitstr

L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:828226 CAPLUS
TITLE: Use of liquid chromatography-mass spectrometry and a chemical cleavage reaction for the structure elucidation of a new sildenafil analogue detected as an adulterant in an herbal dietary supplement
AUTHOR(S): Reepmeyer, John C.; Woodruff, Jeffrey T.
CORPORATE SOURCE: Division of Pharmaceutical Analysis, US Food and Drug Administration, St. Louis, MO, 63101, USA
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (2007), 44(4), 887-893
CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An herbal dietary supplement, marketed as a natural product for the enhancement of sexual function, was analyzed by HPLC with photodiode array and mass spectral detection and found to contain a compound related to the synthetic phosphodiesterase-5 (PDE-5) inhibitors. Based on UV spectra, mass spectra and direct infusion MSn, the structure of the compound was tentatively identified as a sildenafil analog in which the sulfonyl group had been replaced with an acetyl group. This new analog is similar to acetildenafil, a previously reported sildenafil analog, but differs in that it contains an N-Me group where acetildenafil contains an N-Et group. The structure of the unknown was unequivocally established by chemical cleavage of the phenacylamine group of the mol. to generate N-methylpiperazine; other cleavage products matched those generated from acetildenafil. Since the new compound has one less CH2 group than acetildenafil, it was named nor-acetildenafil.

IT 496835-35-9
RL: ANT (Analyte); ANST (Analytical study)
(use of liquid chromatog.-mass spectrometry and a chemical cleavage reaction for structure elucidation of a new sildenafil analog detected as an adulterant in an herbal dietary supplement)
RN 496835-35-9 CAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
(CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS

L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

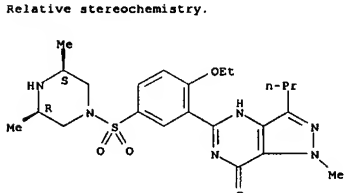
L9 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:646673 CAPLUS
DOCUMENT NUMBER: 147:125726
TITLE: Medicine containing aildenafil for treating sexual impotence
INVENTOR(S): Liu, Baoshun
PATENT ASSIGNEE(S): Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 13pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1977846	A	20070613	CN 2005-10127647	20051206
PRIORITY APPLN. INFO.:			CN 2005-10127647	20051206

AB The title medicine contains aildenafil 15-120 mg (0.1-3 mg/kg body weight), especially 30-120 mg (0.3-3 mg/kg body weight), 30-90 mg/kg (0.3-1.8 mg/kg body weight), and 30-60 mg (0.3-1.2 mg/kg body weight). The dosage form of the medicine can be tablet, capsule, powder, granule, crystal, solution, suspension, syrup, tincture, chewing formulation, nasal spray, nose drop, gel, cream, ointment, emulsion, etc.

IT 496835-35-9
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(medicine containing aildenafil for treating sexual impotence)
RN 496835-35-9 CAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
(CA INDEX NAME)

Relative stereochemistry.



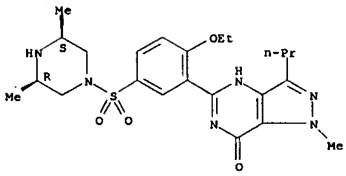
L9 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:422822 CAPLUS
DOCUMENT NUMBER: 147:63259
TITLE: Liquid chromatography tandem mass spectrometry assay to determine the pharmacokinetics of aildenafil in human plasma
AUTHOR(S): Wang, Jiang; Jiang, Yao; Wang, Yingwu; Zhao, Xia; Cui, .
Yimin; Gu, Jingkai
CORPORATE SOURCE: Research Center for Drug Metabolism, College of Life Science, Jilin University, Changchun, 130023, Peop. Rep. China
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (2007), 44(1), 231-235
CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A simple, sensitive and specific liquid chromatog./tandem mass spectrometry method for the quantitation of aildenafil, a new phosphodiesterase V inhibitor, in human plasma is presented. The analyte and internal standard, sildenafil, were extracted by a one-step liquid-liquid extraction in alkaline conditions and separated on a C18 column using ammonia:10mM ammonium acetate buffer:methanol (0.1:15:85, volume/volume/v) as the mobile phase. The detection by an API 4000 triple quadrupole mass spectrometer in multiple-reaction monitoring mode was completed within 2.5 min. The calibration curve exhibited a linear dynamic range of 0.05 - 100 ng/mL with a 10 pg/mL limit of detection. The intra- and inter-day precisions measured as relative standard deviation were within 8.04% and 5.72%, resp. This method has been used in a pharmacokinetic study of aildenafil in healthy male volunteers each given an oral administration of one of the three dosages.

IT 496835-35-9, Aildenafil
RL: BSU (Biological study, unclassified); PKT (Pharmacokinetics); BIOL (Biological study)
(liquid chromatog. tandem mass spectrometry assay to determine the pharmacokinetics of aildenafil in human plasma)
RN 496835-35-9 CAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
(CA INDEX NAME)

Relative stereochemistry.

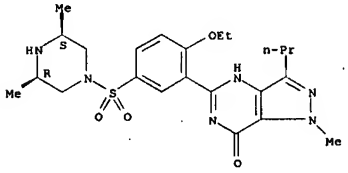
L9 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L9 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:345344 CAPLUS
DOCUMENT NUMBER: 147:39501
TITLE: Structure elucidation of a novel analogue of sildenafil detected as an adulterant in an herbal dietary supplement
AUTHOR(S): Reepmeyer, John C.; Woodruff, Jeffrey T.; 'Avignon, D.
Andre
CORPORATE SOURCE: Division of Pharmaceutical Analysis, US Food and Drug Administration, St. Louis, MO, 63101, USA
SOURCE: Journal of Pharmaceutical and Biomedical Analysis (2007), 43(5), 1615-1621
CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new analog of sildenafil was detected in an herbal dietary supplement, which was sold over the internet and promoted as a product for the enhancement of sexual performance. The structure of the compound was established using LC-MS, UV spectroscopy, MS-MS, and NMR. In addition, the compound was cleaved at its sulfonamide S-N bond yielding a sulfonic acid and an amine, which were independently characterized using LC-MS, GC-MS, and derivatization. The compound, named methisosildenafil, is a novel synthetic analog of sildenafil in which the N-methylpiperazine moiety has been replaced with 2,6-dimethylpiperazine.
IT 496835-35-9, Methisosildenafil
RL: ANT (Analyte); ANST (Analytical study)
(structure elucidation of a novel analog of sildenafil detected as an adulterant in an herbal dietary supplement)
RN 496835-35-9 CAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
(CA INDEX NAME)

Relative stereochemistry.



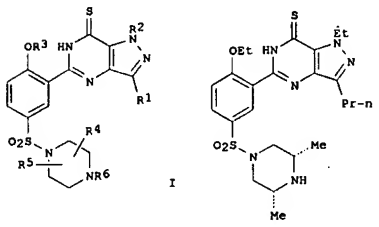
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L9 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:570896 CAPLUS
DOCUMENT NUMBER: 143:97390
TITLE: Preparation of pyrazolopyrimidinethione derivatives for treatment of impotence
INVENTOR(S): Li, Shuxin; Ren, Jianping; Zhao, Yanjin; Lv, Qiujun; Guo, Jinhua
PATENT ASSIGNEE(S): The Institute of Radiation Medicine, Academy of Military Medical Sciences Pla, Peop. Rep. China
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005058899	A1	20050630	WO 2004-CN1312	20041118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1629163	A	20050622	CN 2003-10118481	20031218
EP 1695976	A1	20060830	EP 2004-797343	20041118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
IN 2006MN00737	A	20070330	IN 2006-MN737	20060623
US 2007219220	A1	20070920	US 2007-583335	20070215
PRIORITY APPLN. INFO.:			CN 2003-10118481 A	20031218
			WO 2004-CN1312 W	20041118

OTHER SOURCE(S): CASREACT 143:97390; MARPAT 143:97390
GI

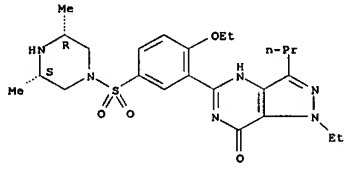
L9 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I II

AB Title compds. represented by the formula I (wherein R1-R3 = independently ((cyclo)alkoxy)alkyl, alkenyl or aryl; R4 = alkyl, alkenyl, (cyclo)alkoxy, aryl; R5 = H, alkyl, alkenyl, (cyclo)alkoxy, aryl; R6 = H, (cyclo)alkyl, alkenyl, alkylcarbonyl; and pharmaceutically acceptable salts or solvates thereof] were prepared for treatment of impotence. For example, II was given in a multi-step synthesis starting from 4-amino-1-ethyl-3-propylpyrazole-5-carboxamide. I showed enhanced erectile response in rats similar to that of Sildenafil. Thus, I and their pharmaceutical compns. are useful for the treatment of impotence and sexlessness, having high selectivity over PDE V, long action time, less side reactions, and no side effects of blood pressure decreasing and heart rate increasing.
IT 856190-55-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolopyrimidinethione derivs. for treatment of impotence)
RN 856190-55-1 CAPLUS
CN Piperazine, 1-[[4-ethoxy-3-(1-ethyl-4,7-dihydro-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)phenyl]sulfonyl]-3,5-dimethyl-, (3R,5S)-rel-
(9CI) (CA INDEX NAME)

Relative stereochemistry.



L9 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

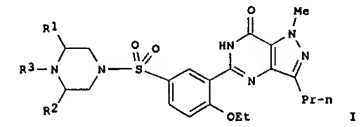
FORMAT

L9 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

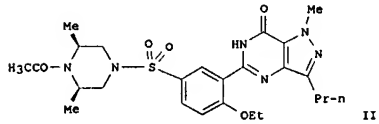
ACCESSION NUMBER: 2005:476529 CAPLUS
DOCUMENT NUMBER: 143:7736
TITLE: Preparation of piperazine derivatives for treating impotence
INVENTOR(S): Liu, Baoshun; Wang, Maotian
PATENT ASSIGNEE(S): Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, No pp. given
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1517349	A	20040804	CN 2003-100488	20030116
PRIORITY APPLN. INFO.:			CN 2003-100488	20030116

OTHER SOURCE(S): CASREACT 143:7736; MARPAT 143:7736
GI



I



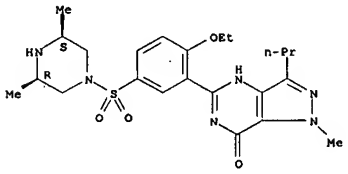
II

AB The title compds. I [wherein R1 and R2 = indepenently alkyl; R3 = acyl or dimethyl] or pharmaceutically acceptable salts or isomers thereof are prepared for the treatment of impotence. For example, the compound II was prepared II showed good result in treating impotence in rat.

IT 496835-35-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of piperazine derivs. for treating impotence)

RN 496835-35-9 CAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
(CA INDEX NAME)

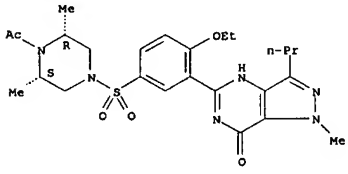
Relative stereochemistry.



IT 852615-88-4P 852615-89-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of piperazine derivs. for treating impotence)

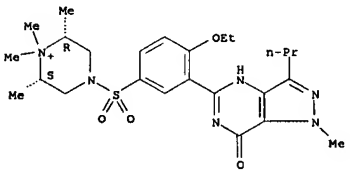
RN 852615-88-4 CAPLUS
CN Piperazine, 1-acetyl-4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-2,6-dimethyl-, (2R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 852615-89-5 CAPLUS
CN Piperazinium, 4-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-1,1,2,6-tetramethyl-, (2R,6S)-rel- (9CI) (CA INDEX NAME)

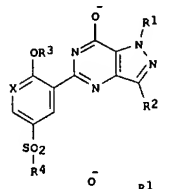
Relative stereochemistry.



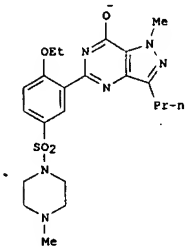
L9 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1009838 CAPLUS
DOCUMENT NUMBER: 142:392422
TITLE: Preparation of fused ring aromatic compounds for treatment of sexual disorders
INVENTOR(S): Lu, Derang; Li, Zhihai
PATENT ASSIGNEE(S): Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 15 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1472210	A	20040204	CN 2002-138880	20020802
PRIORITY APPLN. INFO.:			CN 2002-138880	20020802

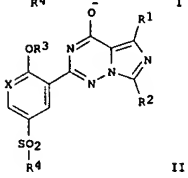
OTHER SOURCE(S): MARPAT 142:392422
GI



I



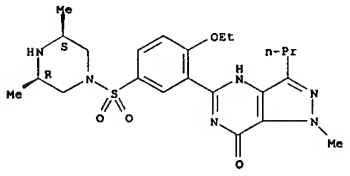
III



II

AB The title compds. I=N+R7R8R9R10 and II=NR7R8R9R10 [wherein R1 = H, alkyl, haloalkyl, or cycloalkyl; R2 = H, (un)substituted alkyl, haloalkyl, or cycloalkyl; R3 = H, (un)substituted alkyl, haloalkyl, cycloalkyl, alkenyl, or alkynyl; R4 = (un)substituted NH2 or piperazinyl; R7, - R10 = independently aryl or alkyl; X = CH or N] are prepared for the treatment of sexual disorders. For example, the compound III=N+Me3(CH2CH2OH) was prepared in a two-step synthesis in good yield. The title compds. showed

L9 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

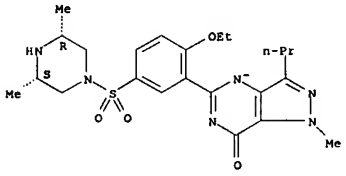


L9 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
strong effect on sexual disorders in rat.
IT 849915-00-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fused ring aromatic compds. for treatment of sexual disorders)
RN 849915-00-0 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with rel-(3R,5S)-1-[[3-(4,7-dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-3,5-dimethylpiperazine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 849914-99-4
CMF C23 H31 N6 O4 S

Relative stereochemistry.



CM 2

CRN 62-49-7
CMF C5 H14 N O

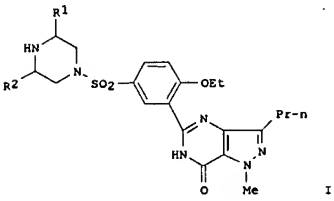
IT 496835-35-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fused ring aromatic compds. for treatment of sexual disorders)
RN 496835-35-9 CAPLUS
CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
(CA INDEX NAME)

Relative stereochemistry.

L9 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:154433 CAPLUS
DOCUMENT NUMBER: 138:153550
TITLE: Preparation of pyrazolopyrimidine derivatives for treatment of impotence
INVENTOR(S): Liu, Baoshun
PATENT ASSIGNEE(S): Peop. Rep. China
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003016313	A1	20030227	WO 2002-CN433	20020621
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1393444	A	20030129	CN 2002-100198	20020118
CN 1127506	B	20031112		
CA 2451990	A1	20030227	CA 2002-2451990	20020621
AU 2002323774	A1	20030303	AU 2002-323774	20020621
EP 1400522	A1	20040324	EP 2002-754139	20020621
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002011025	A	20041019	BR 2002-11025	20020621
JP 2005500381	T	20050106	JP 2003-521235	20020621
NZ 530548	A	20050429	NZ 2002-530548	20020621
RU 2279433	C2	20060710	RU 2004-102513	20020621
HK 1053108	A1	20040402	HK 2003-105310	20030723
US 2004152709	A1	20040805	US 2003-736732	20031216
US 6960592	B2	20051101		
MX 2003PA11929	A	20050307	MX 2003-PA11929	20031218
IN 2003DN02254	A	20060120	IN 2003-DN2254	20031224
ZA 2004000692	A	20041014	ZA 2004-692	20040128
PRIORITY APPLN. INFO.:			CN 2001-129691 A	20010629
			CN 2002-100198 A	20020118
			WO 2002-CN433 W	20020621

OTHER SOURCE(S): CASREACT 138:153550; MARPAT 138:153550
GI



I

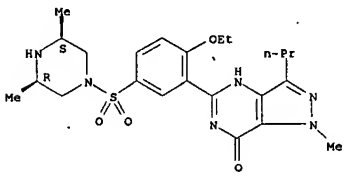
AB Title compound I (R1, R2 = alkyl) and their pharmaceutically acceptable salts or their configuration isomers., useful for treatment of impotence, are prepared Thus, I (R1 = R2 = Me) (II) was prepared in several steps from 2-ethoxybenzoic acid. II showed enhanced erectile response in rats similar to that of sildenafil.

IT 496835-35-9P
RL: ADV (Adverse effect, including toxicity); IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolopyrimidine derivs. for treatment of impotence)

RN 496835-35-9 CAPLUS

CN 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 5-[5-[[(3R,5S)-3,5-dimethyl-1-piperazinyl]sulfonyl]-2-ethoxyphenyl]-1,6-dihydro-1-methyl-3-propyl-, rel-
(CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	45.45	394.18

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.24	-6.24

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:11:40 ON 23 OCT 2007